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Lattice vibrations of α′-NaV2O5

Popova M., Sushkov A., Golubchik S., Mavrin B., Denisov V., Malkin B., Iskhakova A., Isobe M., Ueda Y.

Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

We have measured far infrared reflectance and transmittance spectra as well as Raman scattering spectra of α′-NaV2O5 single crystals for all the principal polarizations. The temperature range above the phase transition temperature Tc = 35 K was investigated, mainly. On the basis of this experimental study and of the lattice dynamics calculations we conclude that the symmetry of NaV2O5 in the high-temperature phase is described by the centrosymmetric D2h 13 space group. This conclusion leads to important physical consequences concerning the interpretation of one-dimensional magnetic properties of NaV2O5 and of the phase transition at 35 K considered earlier to be an ordinary spin-Peierls transition. The assignment of the observed phonons is given. Values of dielectric constants are obtained from the infrared data. Asymmetric shapes of several infrared lines and higher-order infrared vibrational spectra are discussed. The crystal field energy levels of the 3d electron localized at the V4+ site have been calculated in the framework of the exchange charge model using the values of effective charges obtained from the lattice dynamics calculations. According to the results of these calculations, the broad optical bands observed earlier in the vinicity of 1 eV can be interpreted as phonon assisted d-d transitions.